



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 06:12 PM EDT

PDB ID : 6XC4  
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing antibody CC12.3  
Authors : Yuan, M.; Liu, H.; Wu, N.C.; Zhu, X.; Wilson, I.A.  
Deposited on : 2020-06-08  
Resolution : 2.34 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

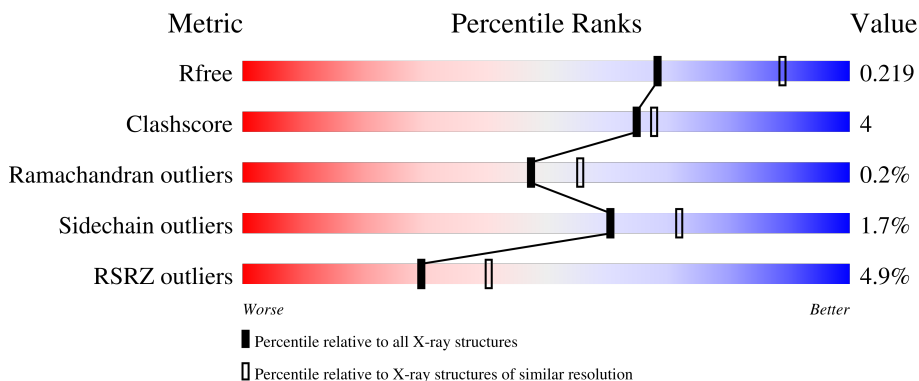
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



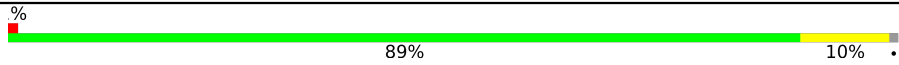
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	 7% 75% 11% 14%
1	Z	231	 13% 74% 10% 16%
2	H	220	 3% 87% 13%
2	X	220	 % 90% 7%
3	L	215	 % 87% 12%

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Mol	Chain	Length	Quality of chain
3	Y	215	 <p>A horizontal bar chart representing the quality of chain. The bar is primarily green, indicating a high quality score of 89%. A small yellow segment at the end indicates a lower quality score of 10%. The bar is labeled with a '%' symbol at the start and '10%' at the end.</p>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10309 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	1575	1008	264	295	8	0	0	0
1	Z	194	1536	985	256	287	8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
Z	542	SER	-	expression tag	UNP P0DTC2
Z	543	GLY	-	expression tag	UNP P0DTC2
Z	544	HIS	-	expression tag	UNP P0DTC2
Z	545	HIS	-	expression tag	UNP P0DTC2
Z	546	HIS	-	expression tag	UNP P0DTC2
Z	547	HIS	-	expression tag	UNP P0DTC2
Z	548	HIS	-	expression tag	UNP P0DTC2
Z	549	HIS	-	expression tag	UNP P0DTC2

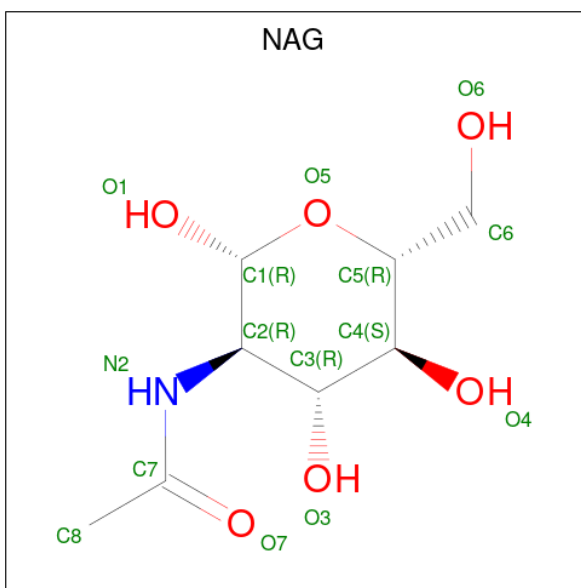
- Molecule 2 is a protein called CC12.3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	220	1645	1040	272	326	7	0	0	0
2	X	214	1606	1019	265	316	6	0	0	0

- Molecule 3 is a protein called CC12.3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	213	Total	C	N	O	S	0	0	0
			1635	1021	279	331	4			
3	Y	213	Total	C	N	O	S	0	0	0
			1635	1021	279	331	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	Z	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	83	Total	O	0	0
			83	83		
5	H	140	Total	O	0	0
			140	140		
5	L	99	Total	O	0	0
			99	99		
5	Z	79	Total	O	0	0
			79	79		

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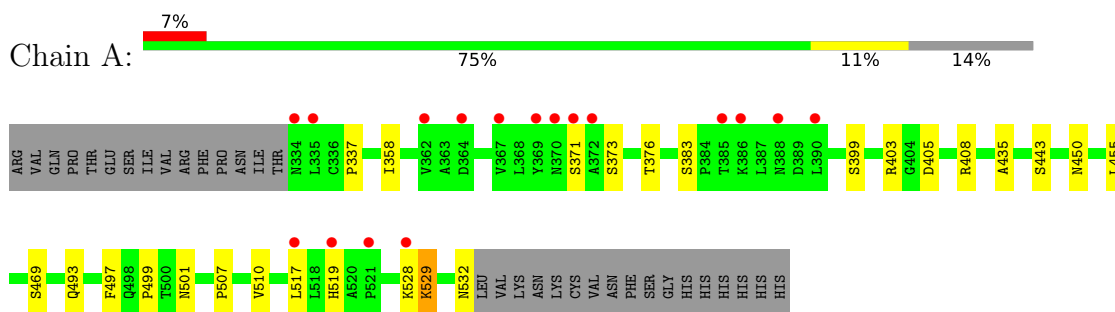
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	X	134	Total 134	O 134	0	0
5	Y	114	Total 114	O 114	0	0

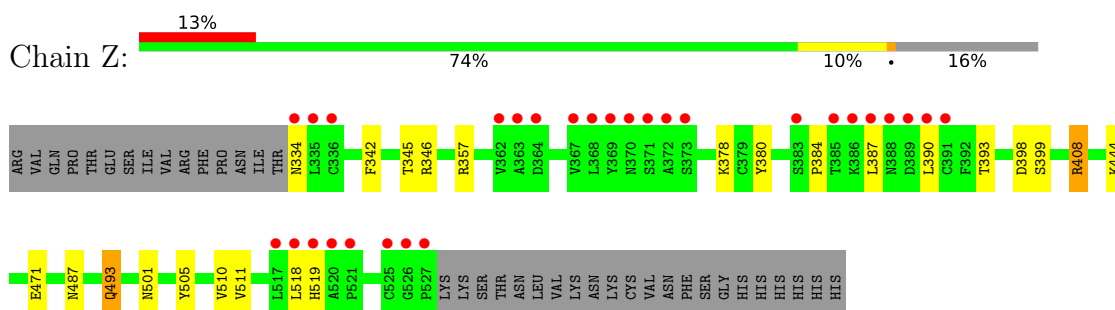
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

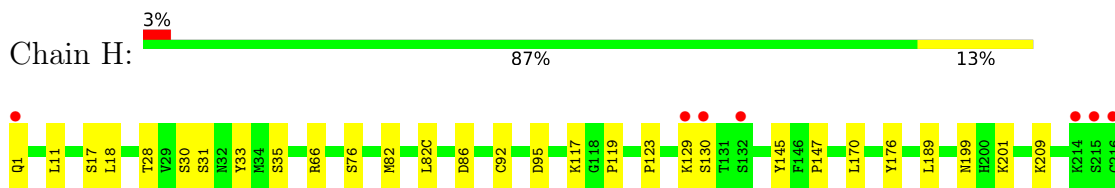
- Molecule 1: Spike protein S1



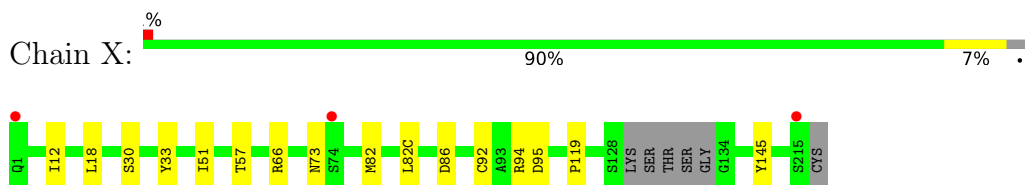
- Molecule 1: Spike protein S1



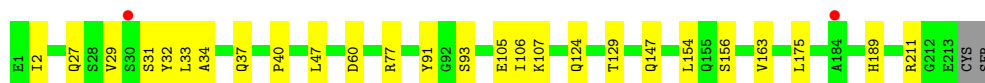
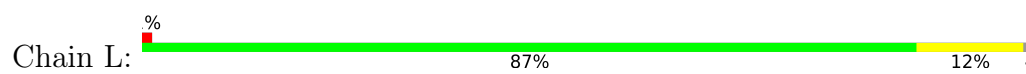
- Molecule 2: CC12.3 heavy chain



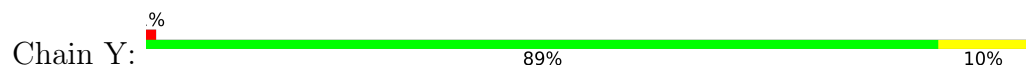
- Molecule 2: CC12.3 heavy chain



- Molecule 3: CC12.3 light chain



• Molecule 3: CC12.3 light chain





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.07Å 105.59Å 165.94Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	41.71 – 2.34 41.71 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.8 (41.71-2.34) 96.8 (41.71-2.34)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.184 , 0.219 0.184 , 0.219	Depositor DCC
$R_{free}$ test set	3800 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtrriage
Anisotropy	0.335	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10309	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/1619	0.47	0/2202
1	Z	0.32	0/1580	0.57	3/2151 (0.1%)
2	H	0.26	0/1685	0.50	0/2292
2	X	0.27	0/1645	0.50	0/2239
3	L	0.27	0/1670	0.52	1/2266 (0.0%)
3	Y	0.31	0/1670	0.56	1/2266 (0.0%)
All	All	0.28	0/9869	0.52	5/13416 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	471	GLU	CA-CB-CG	6.15	126.92	113.40
1	Z	444	LYS	CD-CE-NZ	-5.74	98.50	111.70
1	Z	444	LYS	CB-CG-CD	5.16	125.02	111.60
3	Y	29	VAL	C-N-CA	5.13	134.52	121.70
3	L	29	VAL	C-N-CA	5.09	134.42	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	129	LYS	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1575	0	1496	16	0
1	Z	1536	0	1452	14	0
2	H	1645	0	1604	16	0
2	X	1606	0	1565	8	0
3	L	1635	0	1592	13	0
3	Y	1635	0	1592	12	0
4	A	14	0	13	0	0
4	Z	14	0	13	1	0
5	A	83	0	0	5	0
5	H	140	0	0	4	0
5	L	99	0	0	4	0
5	X	134	0	0	0	0
5	Y	114	0	0	3	0
5	Z	79	0	0	3	0
All	All	10309	0	9327	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 78 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.19	0.75
1:Z:408:ARG:NH2	5:Z:701:HOH:O	2.19	0.74
1:A:371:SER:HG	1:A:373:SER:HG	1.34	0.72
2:H:199:ASN:HD21	2:H:201:LYS:HG2	1.54	0.71
2:X:82:MET:HE2	2:X:82(C):LEU:HD21	1.73	0.69

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/231 (85%)	186 (94%)	11 (6%)	0	100	100
1	Z	192/231 (83%)	183 (95%)	9 (5%)	0	100	100
2	H	218/220 (99%)	213 (98%)	4 (2%)	1 (0%)	29	31
2	X	210/220 (96%)	207 (99%)	3 (1%)	0	100	100
3	L	211/215 (98%)	204 (97%)	6 (3%)	1 (0%)	29	31
3	Y	211/215 (98%)	203 (96%)	7 (3%)	1 (0%)	29	31
All	All	1239/1332 (93%)	1196 (96%)	40 (3%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	130	SER
3	L	31	SER
3	Y	31	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/203 (85%)	168 (98%)	4 (2%)	50	61
1	Z	167/203 (82%)	163 (98%)	4 (2%)	49	59
2	H	186/186 (100%)	183 (98%)	3 (2%)	62	74
2	X	181/186 (97%)	180 (99%)	1 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	184/186 (99%)	181 (98%)	3 (2%)	62	74
3	Y	184/186 (99%)	181 (98%)	3 (2%)	62	74
All	All	1074/1150 (93%)	1056 (98%)	18 (2%)	60	72

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	92	CYS
3	Y	142	ARG
3	Y	93	SER
3	L	93	SER
1	Z	519	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	13	GLN
2	H	199	ASN
1	Z	388	ASN
2	X	1	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.43	0
4	NAG	Z	601	1	14,14,15	0.32	0	17,19,21	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	Z	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Z	601	NAG	O5-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	Z	601	NAG	C4-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	601	NAG	1	0

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	199/231 (86%)	0.42	17 (8%) 10 16	23, 38, 71, 93	0
1	Z	194/231 (83%)	0.68	29 (14%) 2 3	23, 39, 83, 108	0
2	H	220/220 (100%)	-0.05	7 (3%) 47 58	21, 32, 55, 102	0
2	X	214/220 (97%)	-0.10	3 (1%) 75 82	23, 35, 53, 85	0
3	L	213/215 (99%)	-0.04	2 (0%) 84 89	23, 35, 52, 64	0
3	Y	213/215 (99%)	-0.04	3 (1%) 75 82	24, 37, 57, 77	0
All	All	1253/1332 (94%)	0.13	61 (4%) 29 40	21, 35, 68, 108	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	216	CYS	10.4
1	A	372	ALA	6.5
2	X	215	SER	6.1
2	H	215	SER	5.8
1	Z	372	ALA	5.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	601	14/15	0.86	0.25	46,67,77,82	0
4	NAG	Z	601	14/15	0.88	0.27	51,60,70,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.